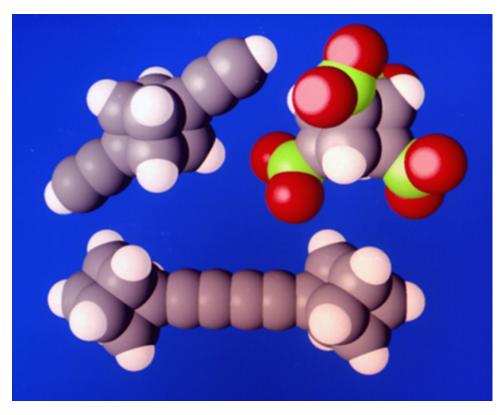
CUBANE CHEMISTRY



Three energetic "cubane" derivatives whose molecular structures were established by single-crystal X-ray analysis at NRL. The compound at top right is tetranitrocubane, a powerful new explosive or propellant ingredient. The other two compounds, containing linear acetylene segments, are rigid-rod molecules called cubylacetylenes.

Cubane is an exotic synthetic hydrocarbon that has eight carbon atoms arranged at the corners of a cube. Bond angle deformations in cubane make it a powerhouse of stored energy. Propellant researchers think that cubane might provide fuels, propellants, and explosives of the future if its chemistry can be mastered. Tetranitrocubane is the most highly nitrated cubane synthesized to date. Preliminary tests indicate that combustion of tetranitrocubane does indeed deliver the extra bond-strain energy predicted by calculations. Cubylacetylenes, also shown, are constructed from cubane and acetylene subunits. They are energetic fuels and "rigid-rod" molecules. Cubylacetylenes are expected to be building blocks in the rapidly developing world of nanoarchitecture, producing organic polymers that are expected to be light, porous, and rigid.

Point of Contact
Naval Research Laboratory
4555 Overlook Avenue, SW • Washington, DC 20375-5320

Richard Gilardi • Laboratory for Structure of Matter • (202) 767-3463 e-mail • gilardi@lsmnic.nrl.navy.mil